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Alloys-by-Design Strategies Using Stochastic Multi-Objective Optimization: Initial Formulation and Results

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13. ABSTRACT (Maximum 200 words)

The objective of this research was to develop and demonstrate a technique for multi-objective optimization of the chemical composition of steel alloys with the use of an existing experimental database. The technique consists in the organization and execution of an iteration optimization experiment, which results in a set of Pareto optimum compositions of steel. The technique is based on the use of algorithms of response surface building known as IOSO. The response surfaces are built in accordance with existing experimental information. In a set of experiments the information on alloy properties in Pareto set neighborhood is accumulated, which makes it possible to increase the accuracy of results obtained. At each iteration of this technique a set of alloy compositions is formed, which are assumed to be Pareto optimal, and for which an experiment should be carried out. For this work, algorithms of artificial neural networks (ANN) were used that utilized radial-basis functions modified in order to build the response surfaces. The modifications consisted in the selection of ANN parameters at the stage of their training that are based on two criteria: minimal curvature of response surface, and provision of the best predictive properties for given subset of test points.

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"Alloys-by-Design Strategies Using Stochastic Multi-Objective Optimization"

Principal Investigator: George S. Dulikravich
Date: January 8, 2003

1. Research objectives

To develop and demonstrate a technique for multi-objective optimization of the chemical composition of an alloy with the use of an existing database.

2. Brief description of technique

2.1. General information

The technique for optimization of the composition of an alloy by a number of criteria consists in the organization and execution of an iteration optimization experiment, which results in a set of Pareto optimum compositions of steel. The technique is based on the use of algorithms of response surface building known as IOSO. The response surfaces are built in accordance with existing experimental information. In a set of experiments the information on alloy properties in Pareto set neighborhood is accumulated, which makes it possible to increase the accuracy of results obtained. At each iteration of this technique a set of alloy compositions is formed, which are assumed to be Pareto optimal, and for which an experiment should be carried out.

During this work, algorithms of artificial neural networks (ANN) were used that utilized radial-basis functions modified in order to build the response surfaces. The modifications consisted in the selection of ANN parameters at the stage of their training that are based on two criteria: minimal curvature of response surface, and provision of the best predictive properties for given subset of test points $W_{best} \in W_{ini}$. Each iteration of alloy composition multi-objective optimization technique involves the following steps:

1. Building and training ANN1 for a given set of test points proceeding from the requirement $W_{best} = W_{ini}$.
2. Conducting multi-objective optimization with the use of ANN1 and obtaining a specified number of Pareto optimal solutions P_1.
3. Determining a subset of test points W_{best} that are maximally close to points P_1 in the space of variable parameters.

4. Training ANN2 proceeding from the requirement to provide the best predictive properties for obtained subset of test points $W_{best} \in W_{ini}$.
5. Conducting multi-objective optimization with the use of ANN2 and obtaining a set of Patero-optimal solutions P_2.

2.2. Features of technique in the presence of an experimental database

In general, the database contains information on experimentally obtained alloy properties compiled from different sources and obtained under different experimental conditions. As a result, for alloys with the same chemical compositions, there can be considerable differences of measured properties. These differences can be explained as errors due to the particular conditions existing during the experiments (measurement errors), and by the effect of certain operating conditions (for example, thermal condition of alloy making). Unless operating conditions are quantified numerically, their influence is regarded as an additional chance factor. In its simplified form the methodology can be presented as the following set of actions:

1. Formulation of optimization task, that is, selection of variable parameters, definition of optimization objectives and constraints, and setting initial (preliminary) ranges of variable parameters variations.
2. Preliminary reduction of the experimental database. At this stage the points meeting optimization task statement are picked up from the database so that alloys having chemical composition outside the chosen set of variable parameters are rejected. Alloys for which there is no data for at least one optimization objective are rejected. In addition, alloys with chemical compositions outside the set range of variable parameters are also rejected.
3. Final reduction of the experimental database. Since accuracy of the building of response surfaces substantially depends on uniformity of distribution of variable parameters in the surveyed area, rejection of experimental data points falling outside of the universal set is performed. At the end of this stage, a final range of variable parameters for optimization is set.
4. Execution of multi-objective optimization resulting in a specified number of Pareto optimal solutions.
5. Analysis of optimization results.
6. Carrying out an experiment to obtain a set of Pareto optimal alloy compositions (or a certain subset) and analysis of the results obtained.
7. Change of optimization problem statement (number of simultaneous objectives and constraints, the set and range of variable parameters), and returning to step 2.
8. Modification of database and returning to step 4.
9. Stop

3. Initial (universal) experimental database

For this particular case, the initial data represented a database containing information on 201 experimentally tested alloys. The data are contained in the file **ini_data.xls**. A preliminary analysis of data has shown that for certain alloys there is no complete information on alloy chemical composition. Such alloys were excluded from further analysis. Besides, some chemical elements (***V, Bi, Se, Zr, Sb, Cd*** **)** were present in a very small number of alloys, which makes it impossible to assess their effect proceeding from information in this database. Such alloys were also excluded from further analysis. The remaining database had 176 alloys (file **first.xls**).

At the next stage, an evaluation of uniformity of distribution of the percentage values of different elements in the existing range was made. It turned out that certain alloys had percentages differing very strongly from the universal set. As an example Fig.1 presents distribution of the percentage of sulfur in the alloys of the reduced database. The alloy No.67 had percentage of sulfur exceeding average value by some 10 times. Such alloys were excluded from further analysis. The capacity of the remaining database was 158 alloys (the file **second.xls**).

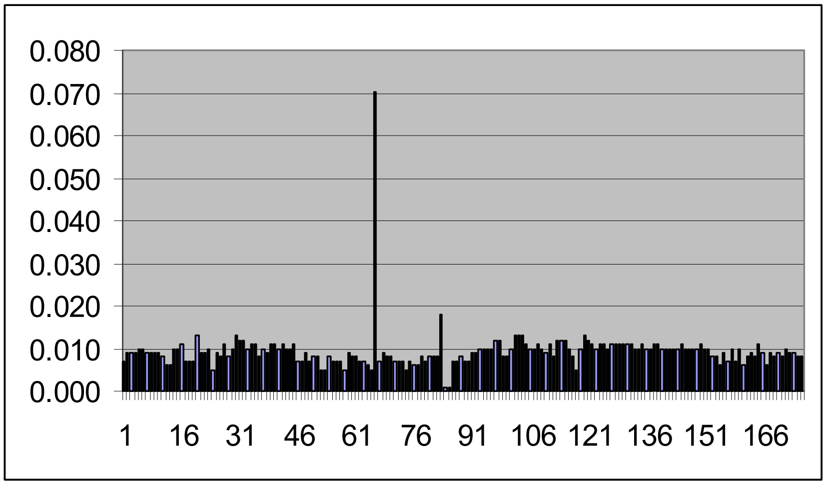


Fig. 1. Distribution of percentage of sulfur (S) in database alloys.

4. Features of optimization problem statement

4.1. Variable parameters

In this problem the percentages of the following 17 elements were taken as independent variables: ***C, S, P, Cr, Ni, Mn, Si, Cu, Mo, Pb, Co, Cb, W, Sn, Al, Zn, Ti***.

The ranges of these elements were set as follows. First, minimum and maximum values for existing set of experimental data ($Exp\_min_i, Exp\_max_i,\ i = \overline{1,17}$) were defined. Then, new minimum and maximum values for each of the 17 elements were obtained according to the following simple dependencies: ($Min_i = 0.9 \cdot Exp\_min_i, Max_i = 1.1 \cdot Exp\_max_i,\ i = \overline{1,17}$). The existing ranges are given in Table 1.

Table 1. Ranges of variation of independent variables

	C	S	P	Cr	Ni	Mn	Si	Cu	Mo
min	0.063	0.001	0.009	17.500	19.300	0.585	0.074	0.016	0.000
max	0.539	0.014	0.031	39.800	51.600	1.670	2.150	0.165	0.132

	Pb	Co	Cb	W	Sn	Al	Zn	Ti
min	0.001	0.000	0.000	0.000	0.000	0.001	0.001	0.000
max	0.006	0.319	1.390	0.484	0.007	0.075	0.015	0.198

4.2. Optimization objectives

The following parameters were used as optimization objectives:

- Stress (PSI – maximize);
- Operating temperature (T – maximize);
- Time to "survive" until rupture (Hours – maximize).

Under the research the solution of a three-objectives optimization problem and a series of two-objectives problems were accomplished when one of the considered parameters was constrained.

5. Obtained results

5.1. Problem No. 1.

During the first stage, the problem of three-objectives optimization was solved with 100 points of Pareto optimal solutions. The results are given in the file **task1.xls**. Figure 2 presents obtained Pareto optimal solutions in objectives' space (PSI – HOURS). Analysis of this figure allows us to extract an area of admissible combinations of different optimization objectives. It can be seen that results are distributed in the admissible part of the objectives' space quite uniformly. Such a distribution offers a possibility for a significant improvement of accuracy of response surfaces on condition that the experiments will be carried out at the obtained Pareto optimal points. In principle, the first iteration of the process of alloy chemical composition optimization by several objectives could be regarded as completed. Then, in accordance with the elaborated technique, it is necessary to conduct experiments at the obtained Pareto optimal points, evaluate accuracy of prediction of values of partial optimization criteria, and either complete the process or perform another iteration.

However, such a strategy seems very difficult to implement for a researcher who knows his tasks more accurately. It can be seen that the ranges of variation of optimization objectives for obtained Pareto set are very wide. At the same time, if a researcher can formulate the problem more specifically (for example, by setting constraints on the objectives) the volume of experimental work can be substantially reduced.

Figure 3 and Figure 4 presents interdependence of the chosen optimization objectives built on the obtained set of Pareto optimal solutions. Analysis of these figures shows that the increase of temperature, for instance, leads to the decrease of compromise possibilities between PSI and HOURS. Hence, if a researcher knows exactly in what temperature range the alloy being designed will be used, it is more economical that the problem of two-objectives optimization be solved with additional constraint for the third efficiency parameter.

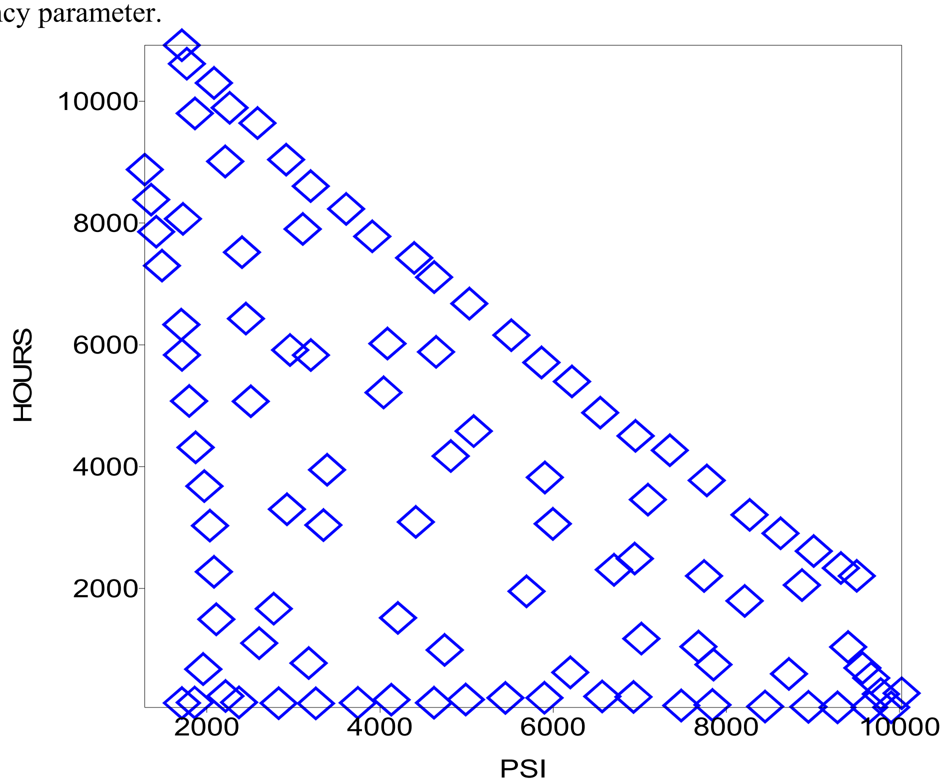


Fig.2. Results of Problem No.1 solution in objectives' space.

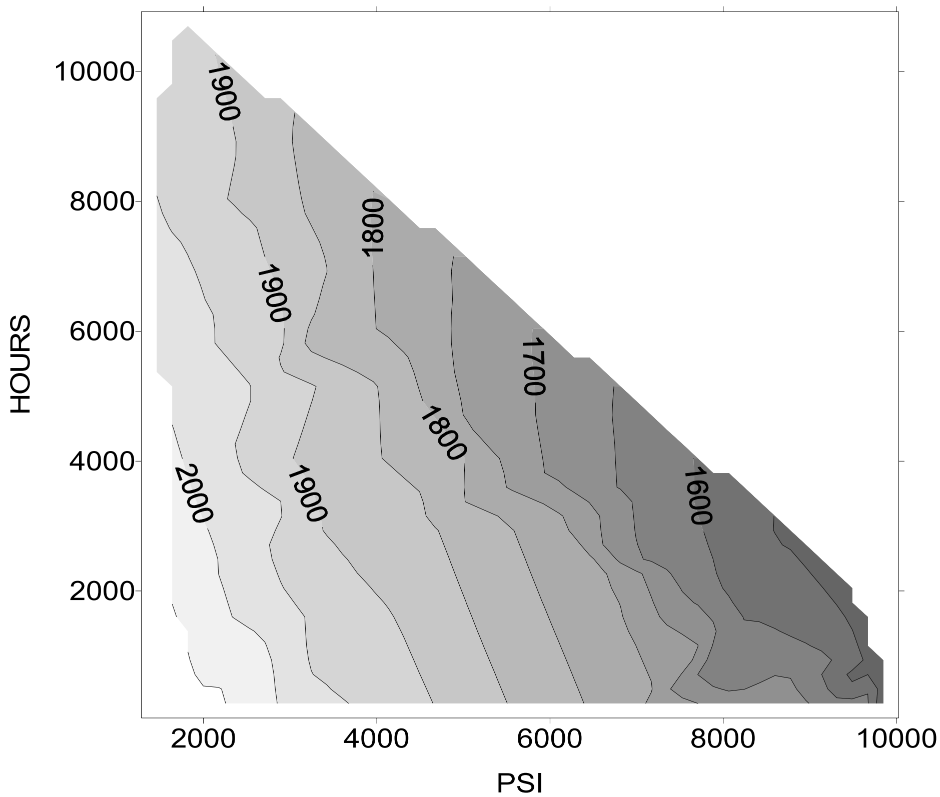


Fig.3. Time to rupture vs. strength interdependence of optimization objectives for Pareto set.

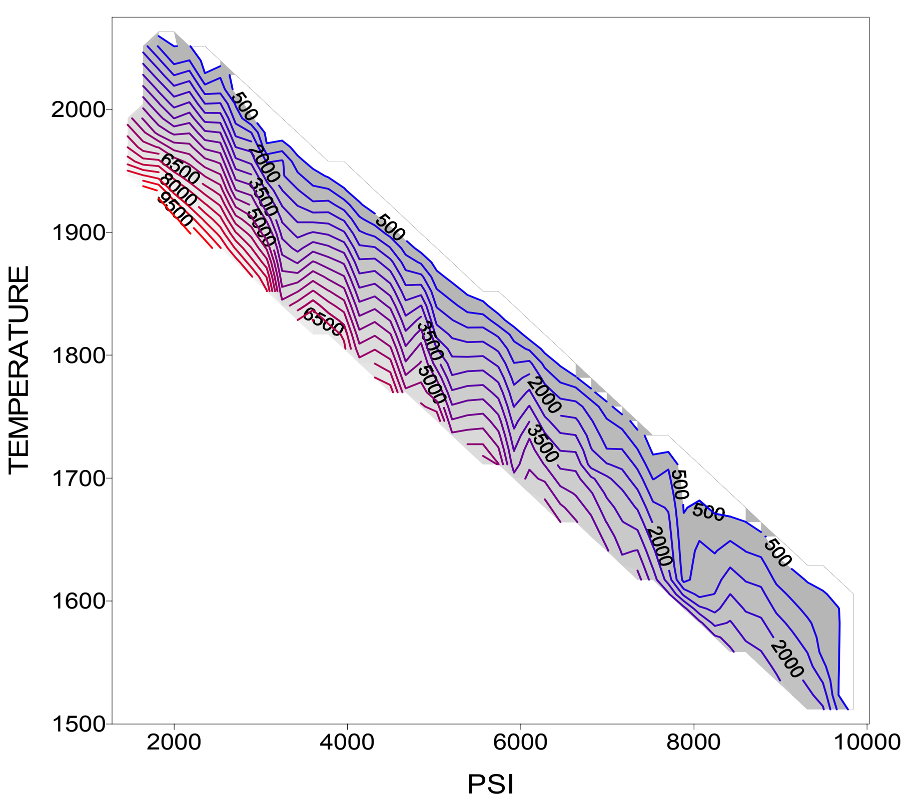


Fig.4. Temperature vs. strength iterdependence of optimization objectives for Pareto set.

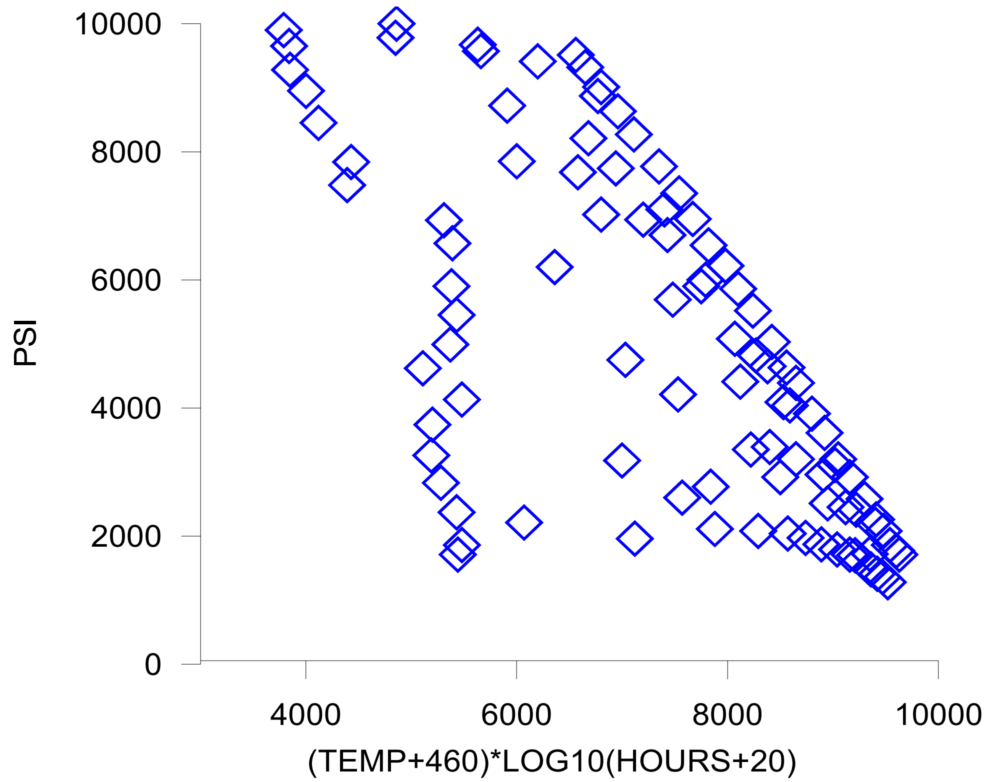


Fig. 5. Larsen-Mueller diagram for 3-criteria optimization results.

Larsen-Mueller diagram (Fig. 5) has PSI on the vertical axis and the following expression on the horizontal axis (Temperature in Rankine degrees) * log(HOURS + 20). Here, logarithm is with the basis 10, while temperature is in Rankine = temperature in Fahrenheit + 460.

5.2. Problems No.2

This part presents results of solution of five additional two-objectives problems in which PSI and HOURS were regarded as simultaneous objectives, and different constraints were placed on temperature:

- Problem 2. - $T \geq 1600$, number of Pareto optimal solutions is 20.
- Problem 3. - $T \geq 1800$, number of Pareto optimal solutions is 20.
- Problem 4. - $T \geq 1900$, number of Pareto optimal solutions is 20.
- Problem 5. - $T \geq 2000$, number of Pareto optimal solutions is 15.
- Problem 6. - $T \geq 2050$, number of Pareto optimal solutions is 10.

Results of solution of these problems are contained in the file **task2-6.xls**. Some of the graphical results are presented in Figs. 6-10.

Figure 6 presents obtained sets of Pareto optimal solutions in objectives space. It can be seen that maximum achievable values of PSI and HOURS, and possibilities of compromise between these parameters largely depend on temperature. For instance, the increase of minimum temperature from 1600 F to 1900 F leads to the decrease of attainable PSI by more than 50 percent. At the same time, limiting value of HOURS will not alter with the change of temperature.

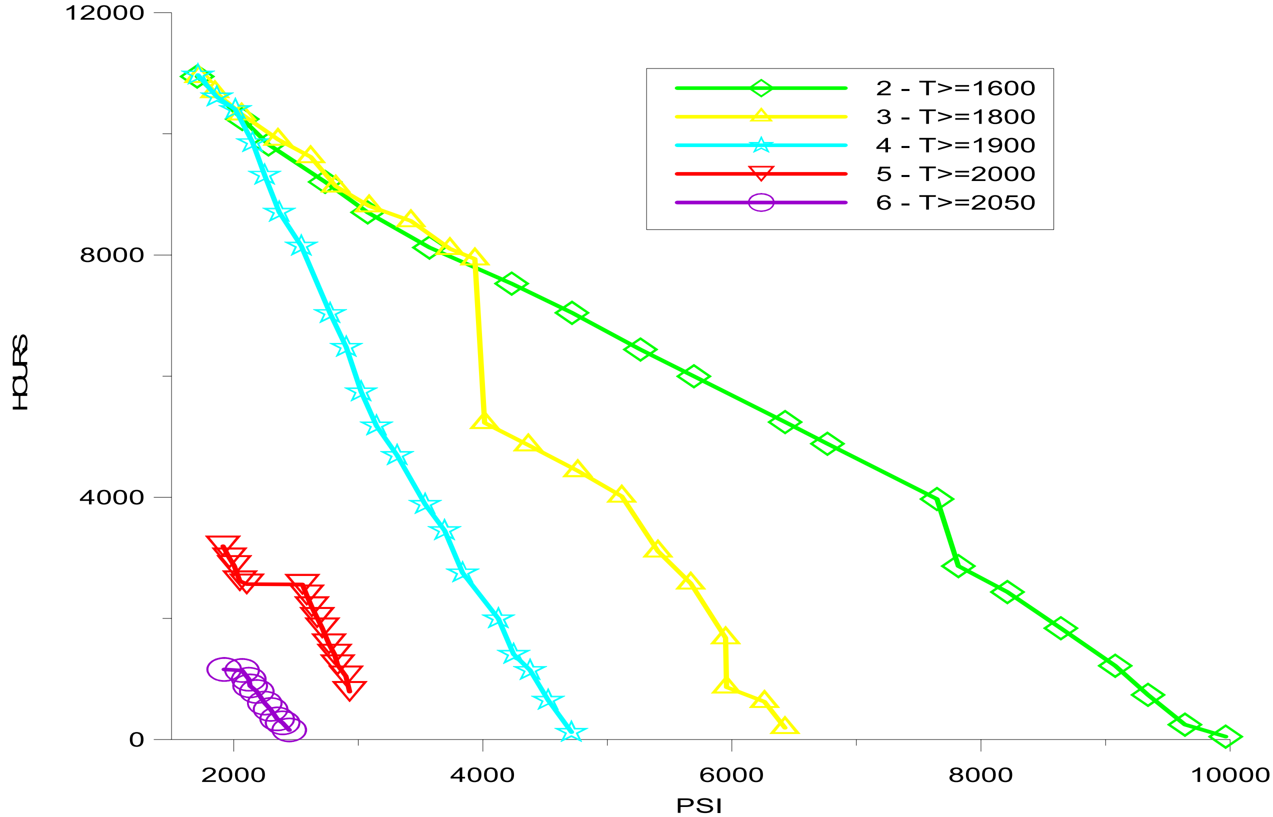


Fig. 6. Sets of Pareto optimal solutions of five problems with 2-objectives.

The decrease of the number of simultaneous optimization objectives (transition from three- to two-objectives problem with constraints) leads to the decrease of the number of additional experiments needed, at the expense of both decreasing the number of Pareto optimal points and decreasing the ranges of chemical compositions.

Three-dimensional plots (Pareto surfaces) where the three coordinates are PSI, TEMP, and HOURS are given in Figures 7 and 8. Notice that since the range of Pareto-optimal points distribution is not a square, the quality of the surfaces is somewhat reduced:

Larsen-Mueller diagram for this set of cases (2-objective optimization for five temperatures) is shown in Figure 9.

We also calculated sensitivity derivatives at 7 Pareto-optimal points. These derivatives are in the "***derivatives.xls***" file. But we think, that accuracy of these evaluations is very low.

Figs. 10-13 show ranges of percentages of different elements for initial set of experimental data, and for results of solution of six optimization problems. It is noteworthy that a competent analysis of results obtained can allow the specialist to soundly choose chemical compositions for which the experiment is necessary, from the viewpoint of achieving desirable values of optimization objectives and building a more accurate response surface.

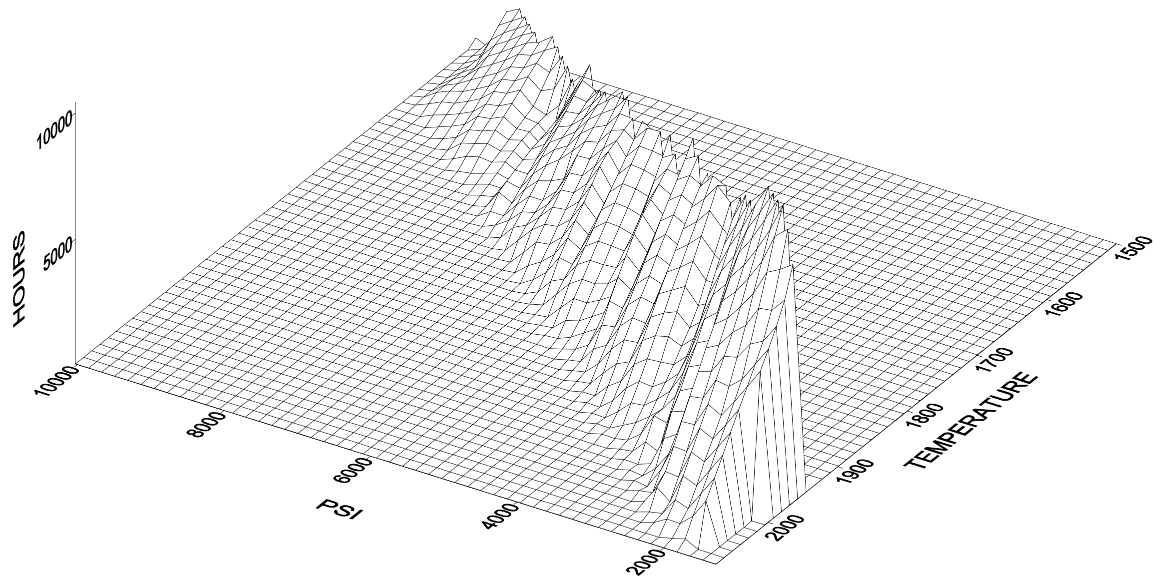


Fig. 7. Non-cumulative plots showing T=2050, T=2000, T=1900, T=1800, T=1600.

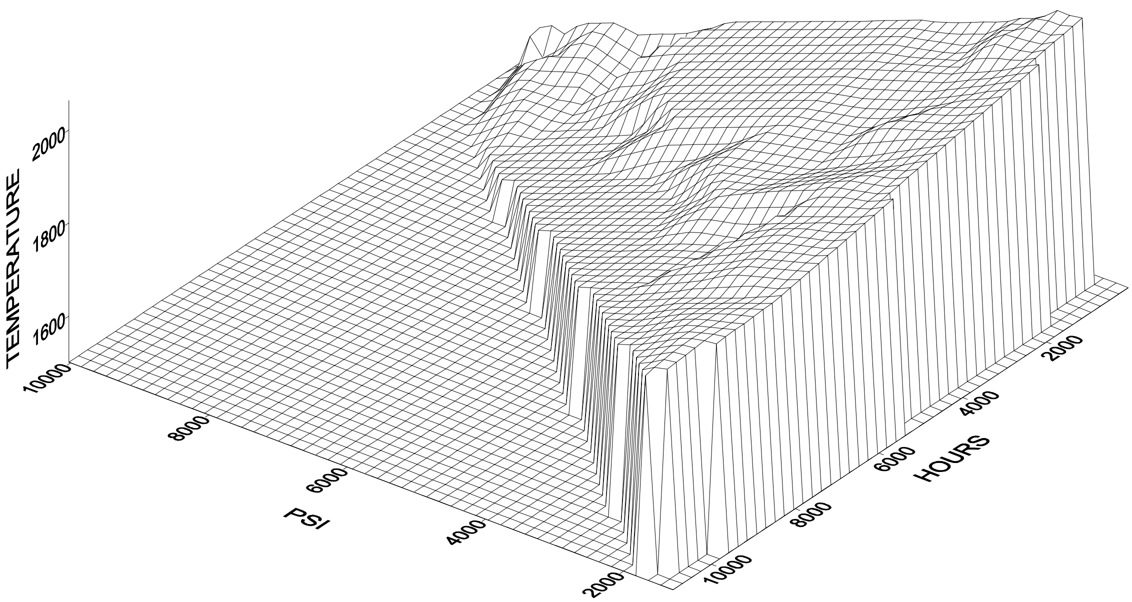


Fig. 8. Non-cumulative plots showing T=2050, T=2000, T=1900, T=1800, T=1600.

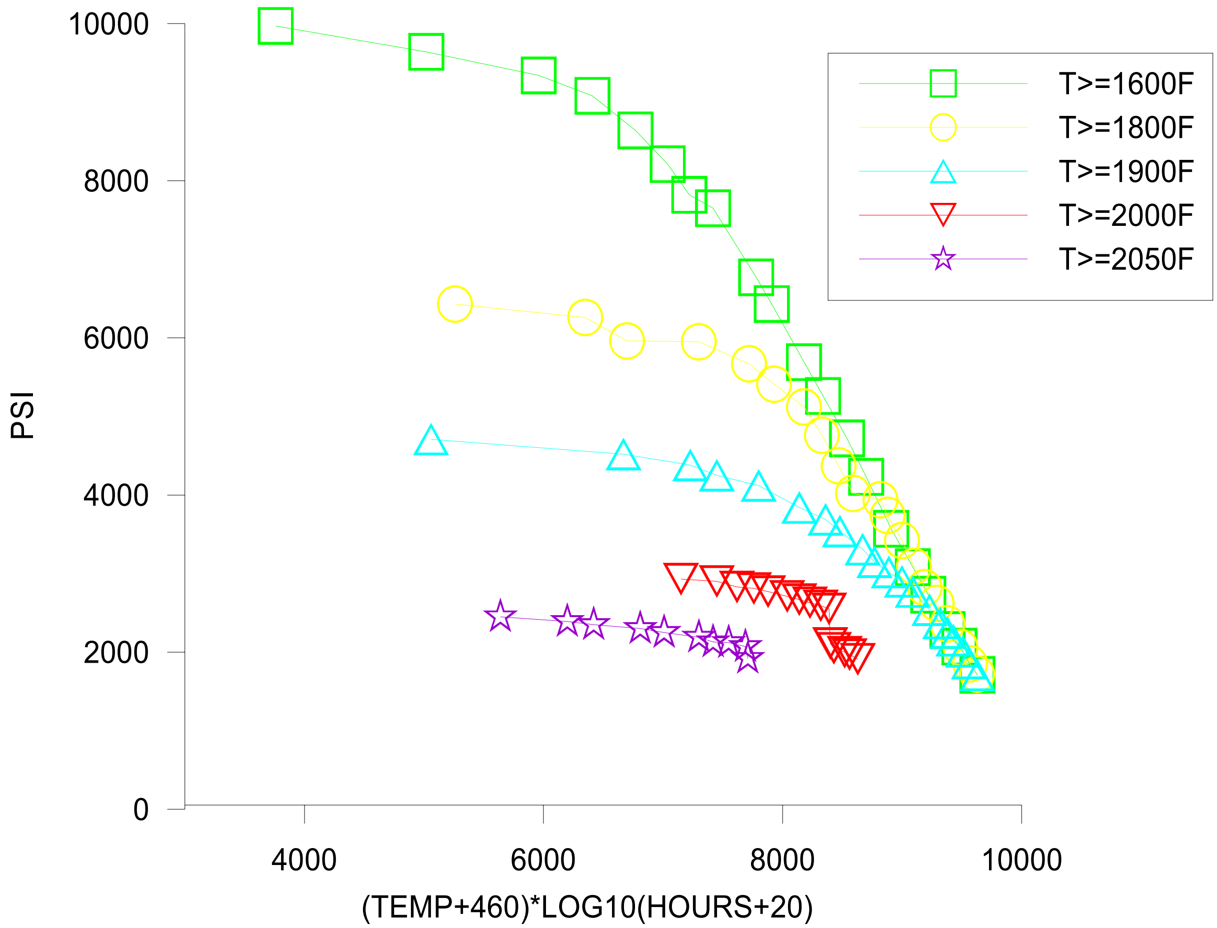


Fig. 9. Larsen-Mueller diagrams for five 2-criteria optimization problems results.

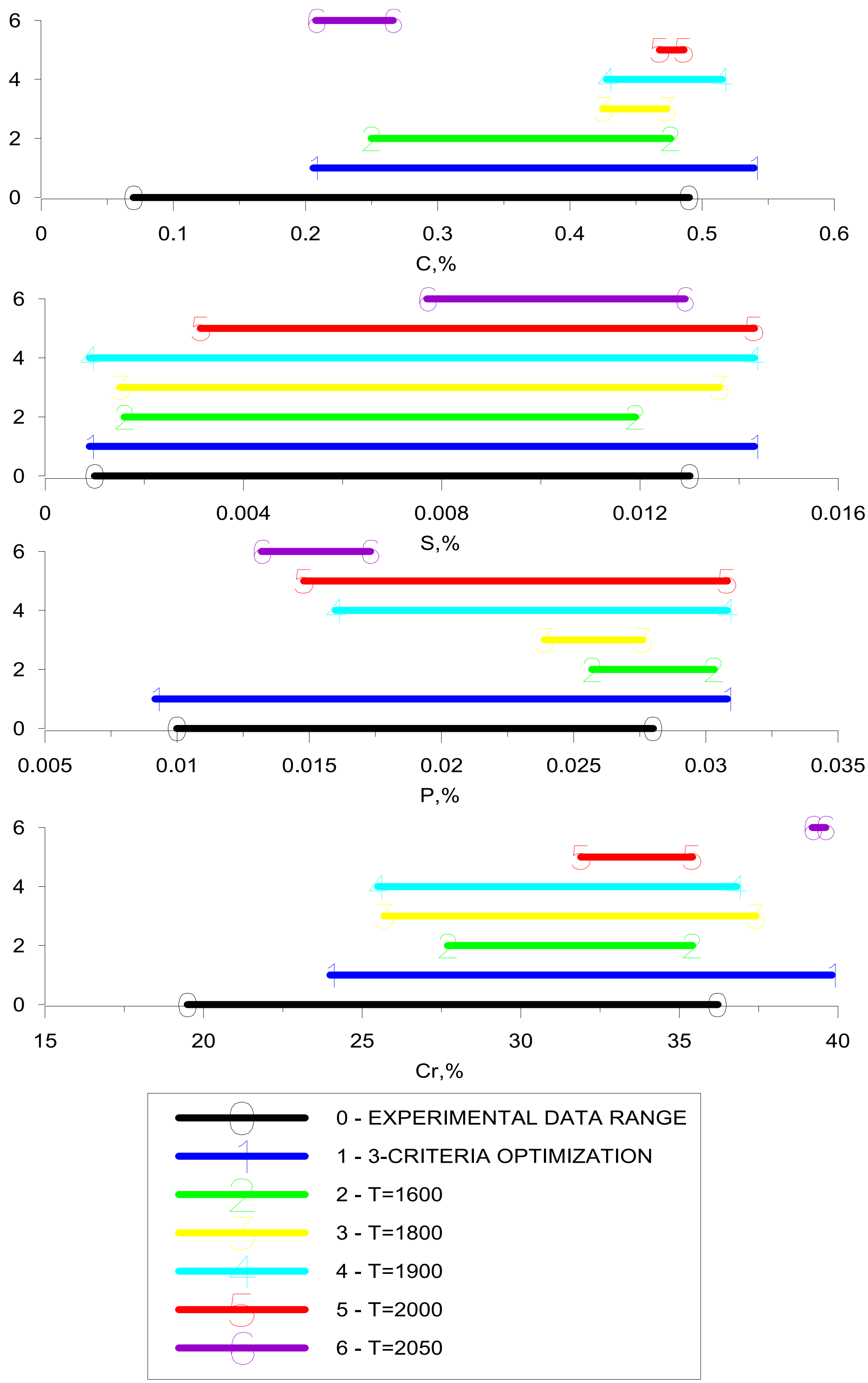


Fig. 10. Boundaries of variable parameters for sets of Pareto optimal solutions.

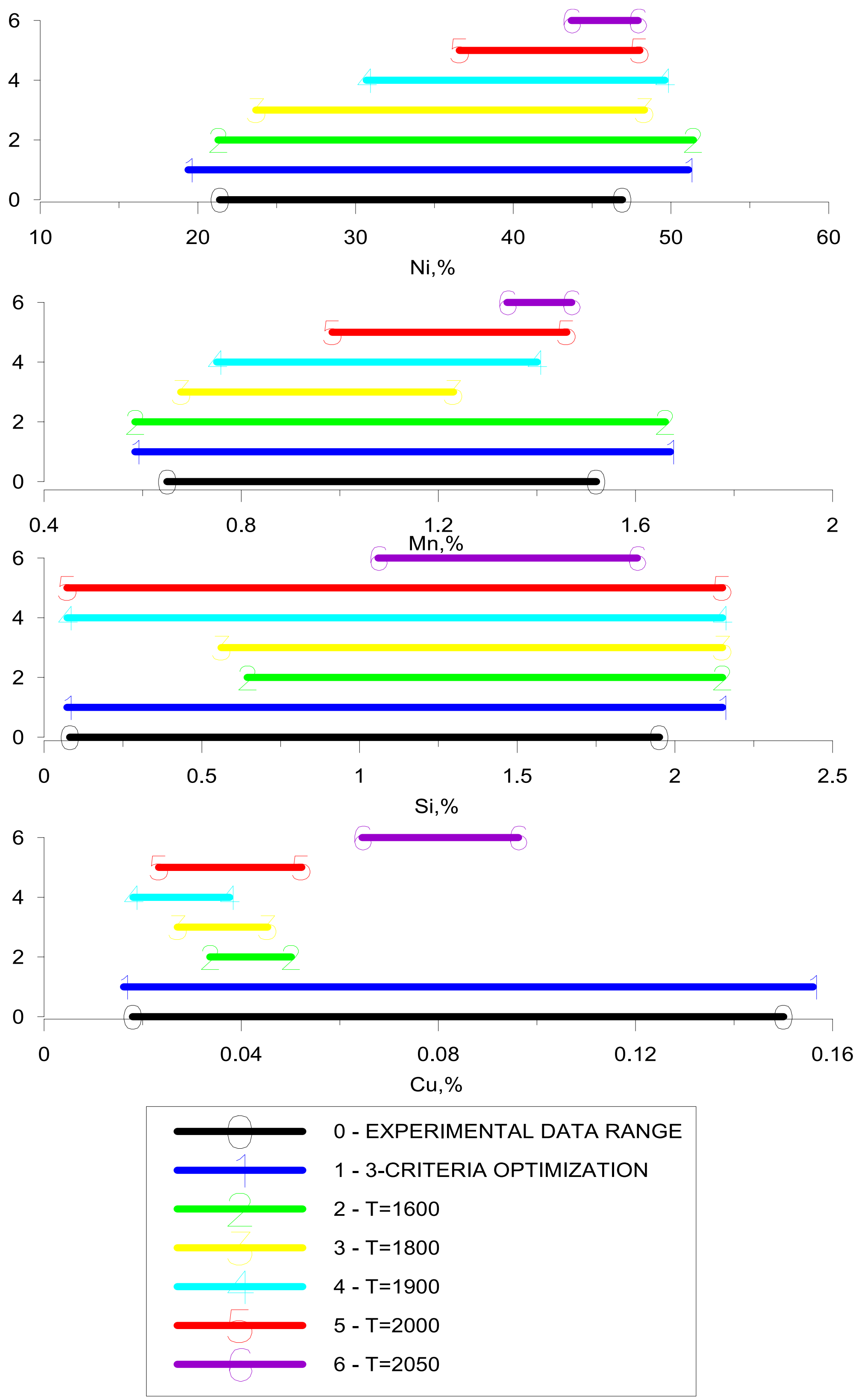


Fig. 11. Boundaries of variable parameters for sets of Pareto optimal solutions.

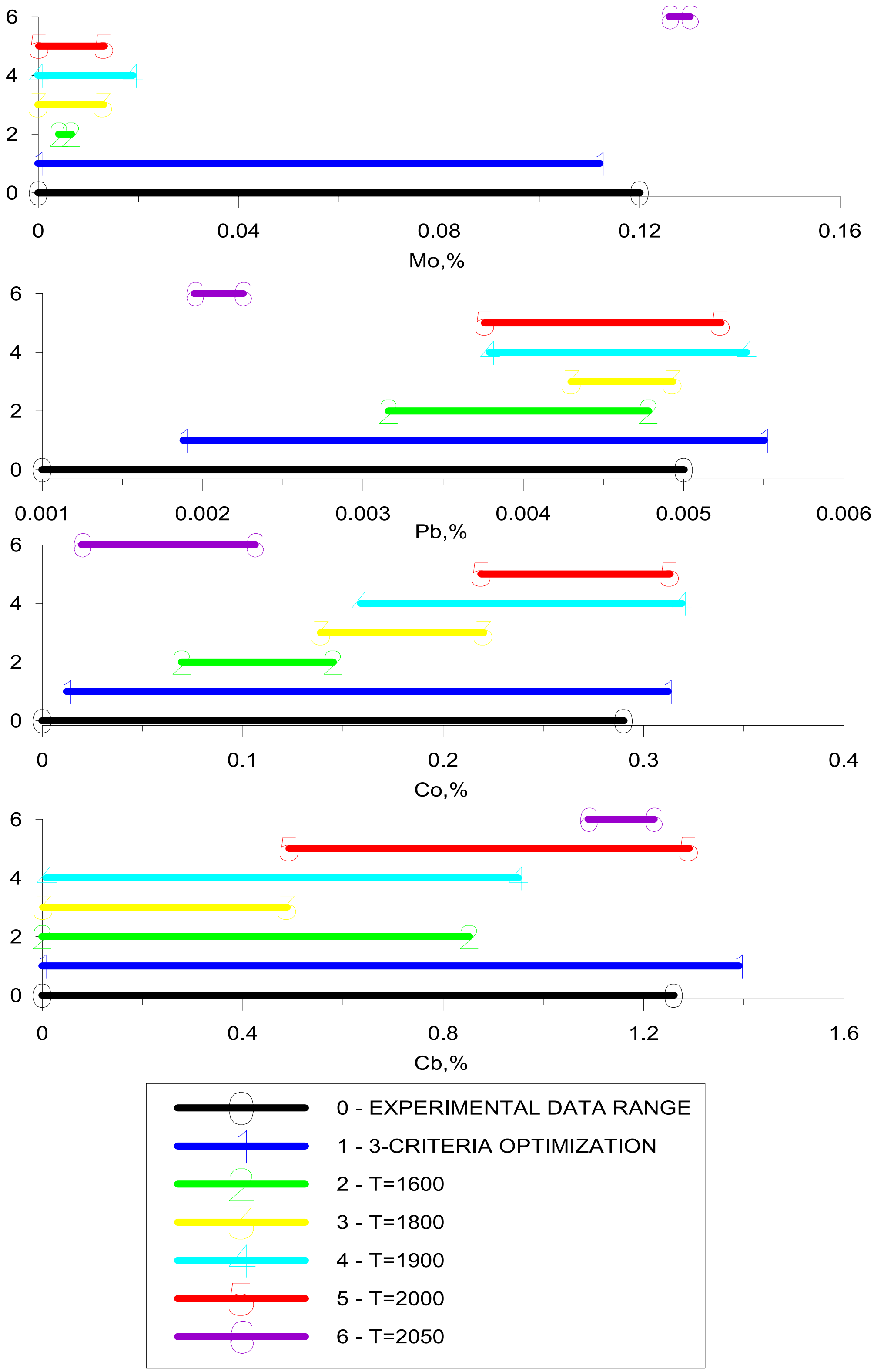


Fig. 12. Boundaries of variable parameters for sets of Pareto optimal solutions.

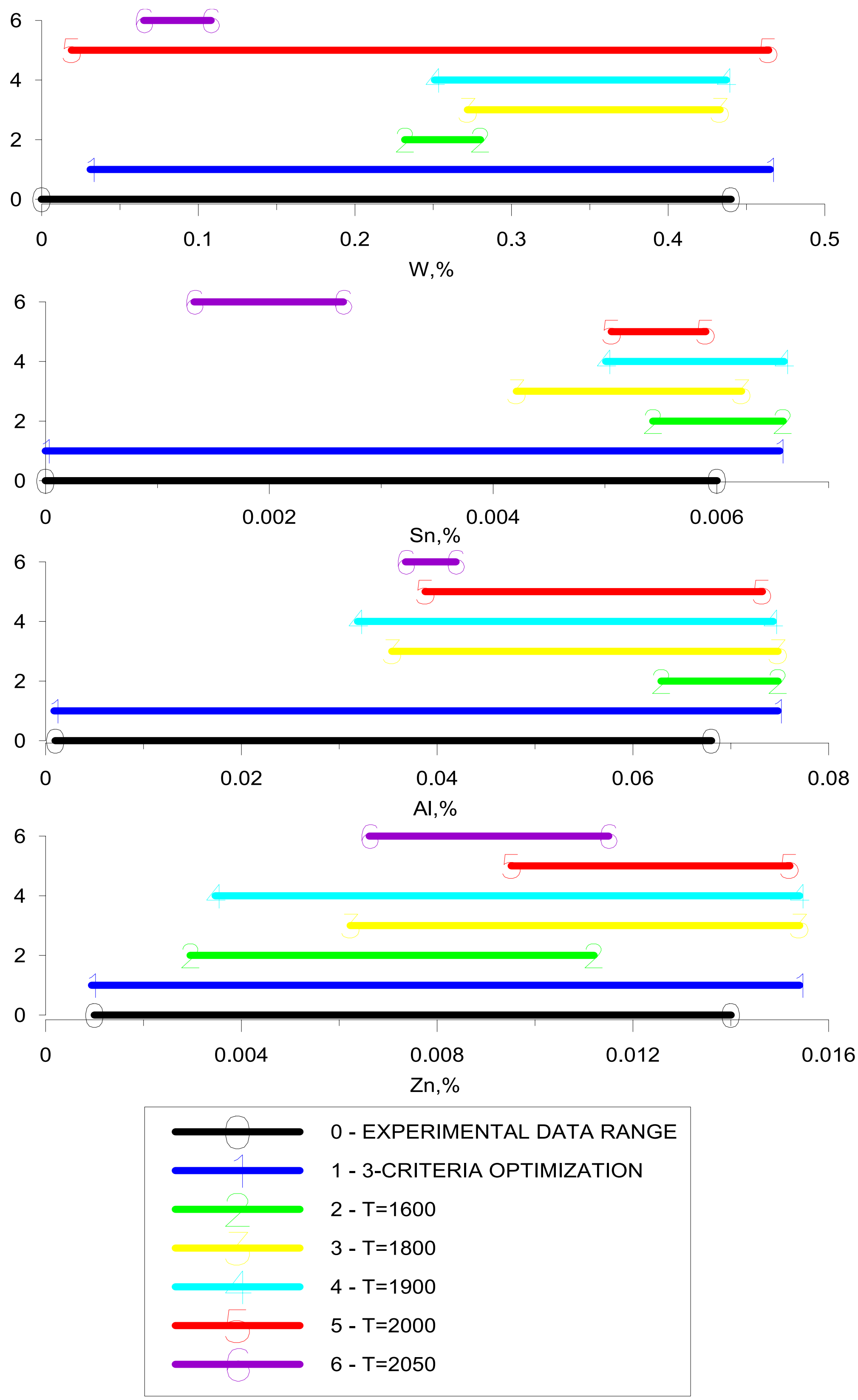


Fig. 13. Boundaries of variable parameters for sets of Pareto optimal solutions.

OPTIMIZATION RESULTS FOR THE CASES WITH 9 DESIGN VARIABLES

We then repeated the three-objectives optimization run in which we used only the following 9 chemical elements as independent variables:

C, Cr, Ni, Mn, Si, Mo, Cb, W, Ti.

We have followed the same steps during the optimization as when solving the problem with 17 variables. But, in this case there are differences:

1) The variables' ranges were changed.
In these tables you can see the previous ranges and the current ranges.

Table 1. Ranges of variation of independent variables (problem with 17 variables)

	C	S	P	Cr	Ni	Mn	Si	Cu	Mo
min	0.063	0.001	0.009	17.500	19.300	0.585	0.074	0.016	0.000
max	0.539	0.014	0.031	39.800	51.600	1.670	2.150	0.165	0.132

	Pb	Co	Cb	W	Sn	Al	Zn	Ti
min	0.001	0.000	0.000	0.000	0.000	0.001	0.001	0.000
max	0.006	0.319	1.390	0.484	0.007	0.075	0.015	0.198

Table 2. Ranges of variation of independent variables (problem with 9 variables)

	C	Cr	Ni	Mn	Si	Mo	Cb	W	Ti
min	0.00	17.50	25.00	0.00	0.00	0.00	0.00	0.00	0.00
max	0.60	30.00	35.00	2.00	2.00	2.00	3.00	2.00	2.00

2) The accuracy of response surfaces deteriorates.
The main reason of accuracy deterioration is that while decreasing the number of variables for the same experimental data set, we added the additional noise. For example, in the file "DISTAN.XLS" you can find five pairs of points that are very close in variable space, but have a drastically different values of objectives.

3-criteria optimization using 9 design variables (chemical species).

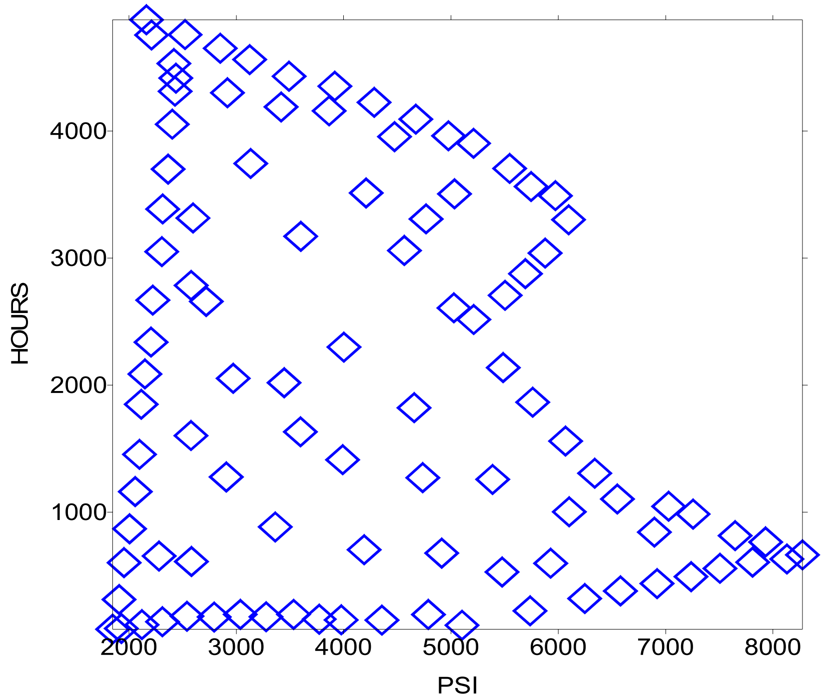
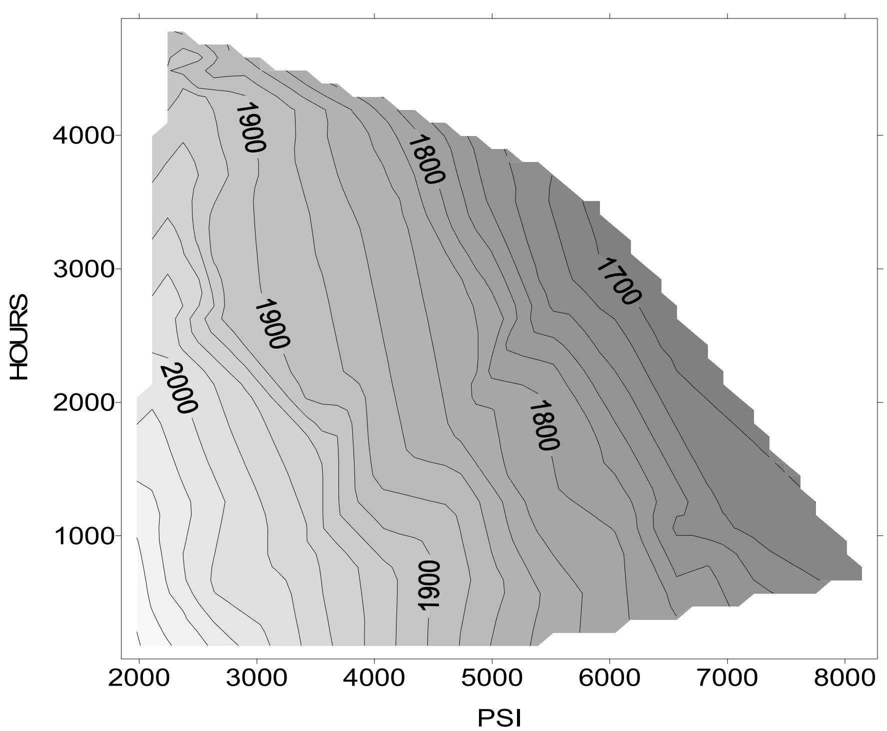


Fig.1. Distribution of points in objectives space using 9 design variables (chemical species).



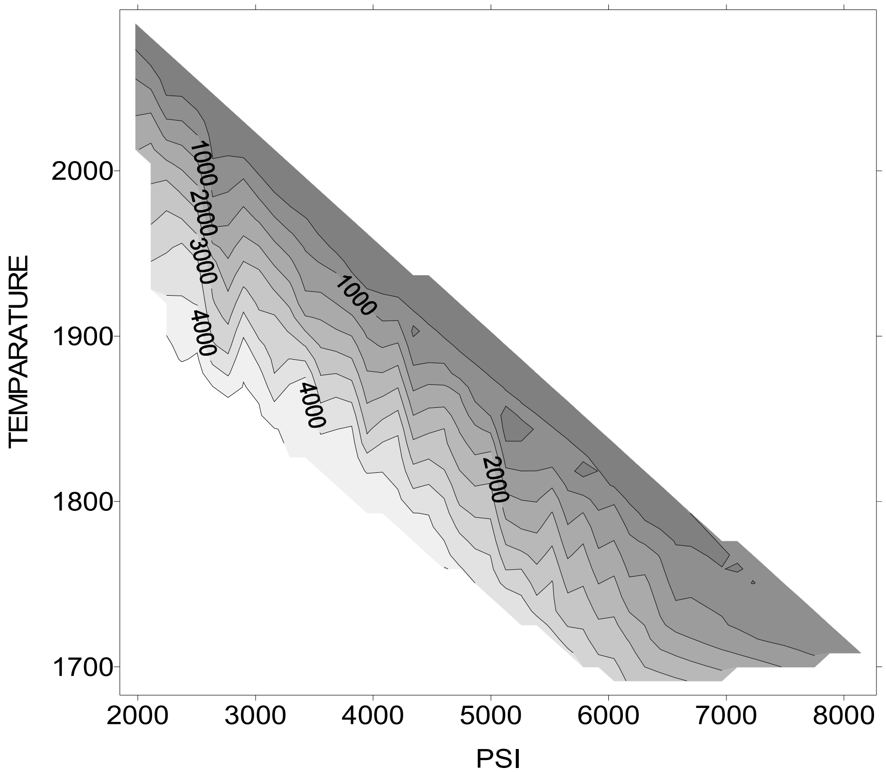
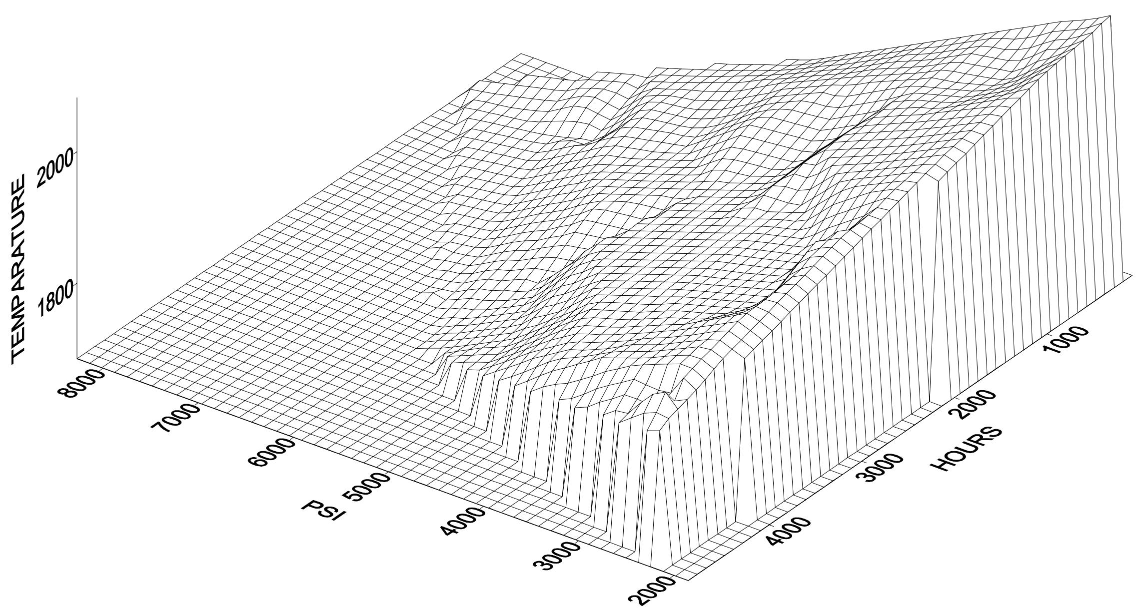


Fig.2. Interdependence of optimization objectives for Pareto set using 9 design variables (chemical species).



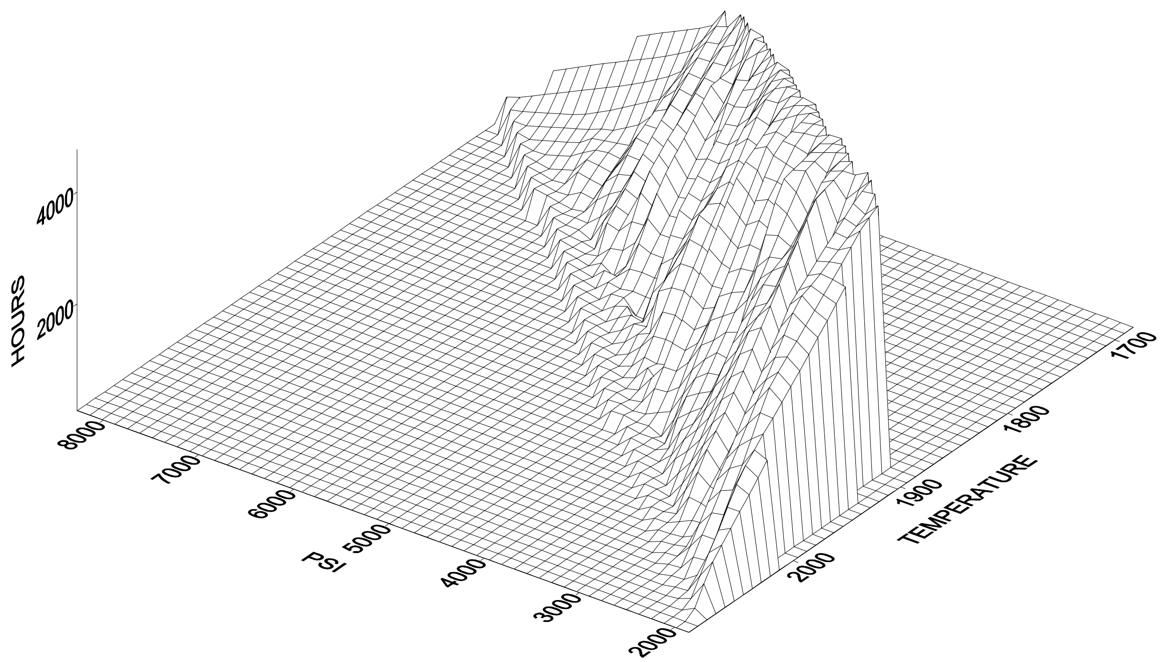


Fig.3. Pareto surfaces using 9 design variables (chemical species).

2-objectives optimization using 9 design variables (tasks N2,…,N6).

Analysis of the 3-criteria optimization results shows that there are no solutions with temperature less or equal 1600F. Because of this, we changed the value of a constraint for the task N2. Constraint $T \geq 1600$ was replaced with $T \geq 1700$.

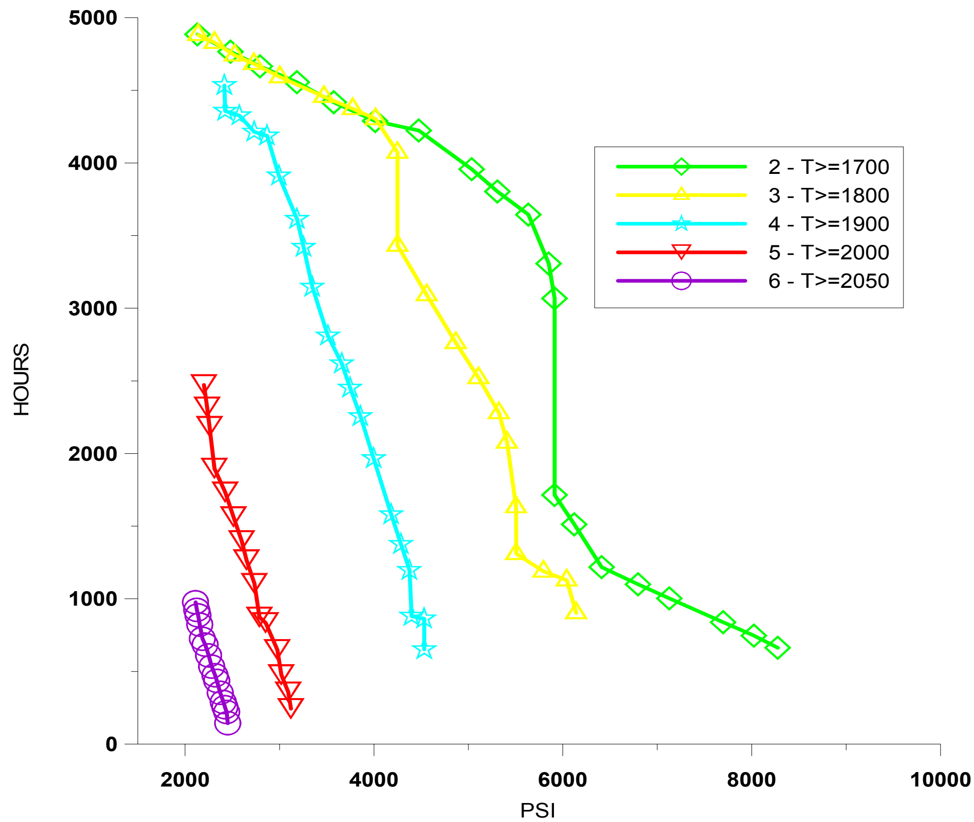


Fig.4. Pareto-optimal sets for five different (temperature) constraints using 9 design variables.

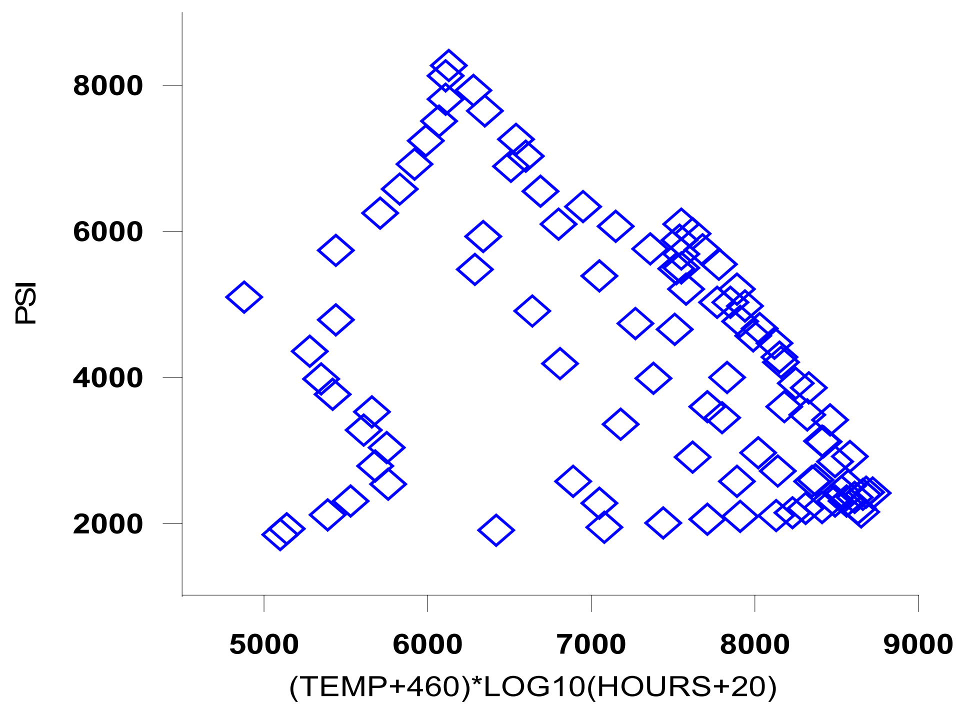


Fig. 5. Larsen-Mueller diagrams for 3-criteria optimization problems using 9 design variables.

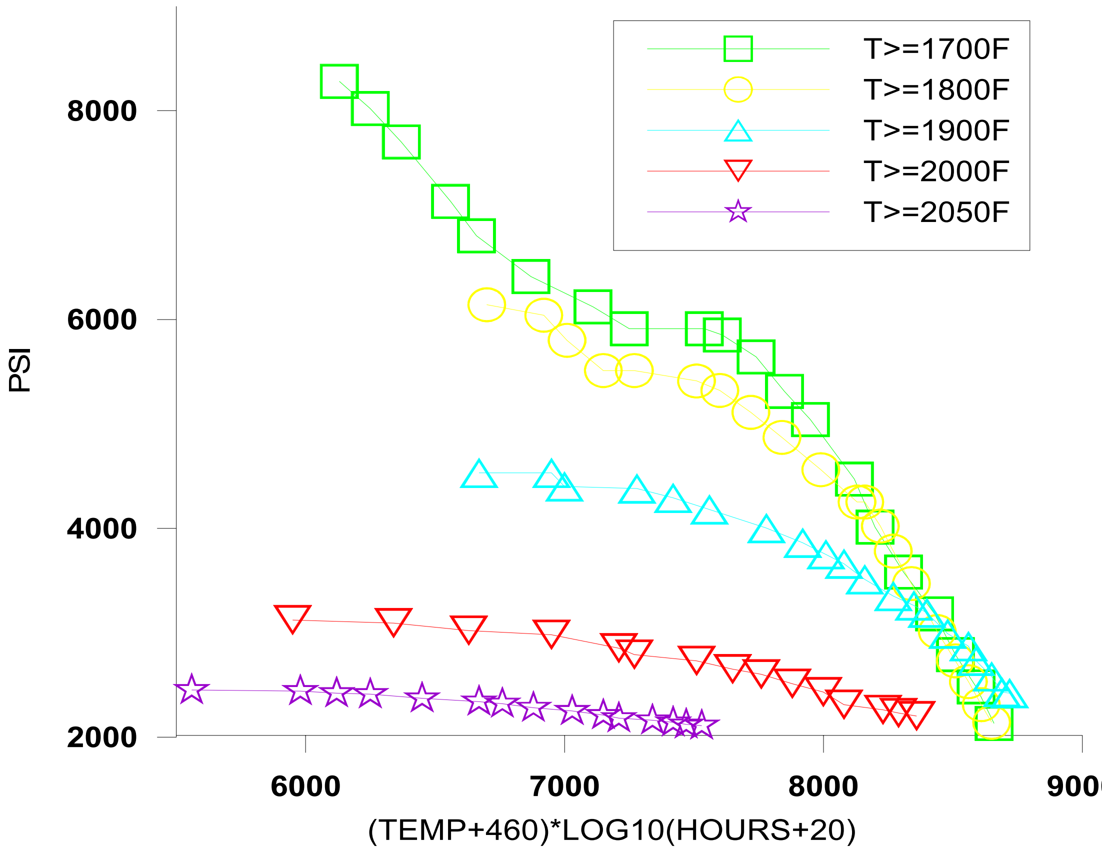


Fig. 6. Larsen-Mueller diagrams for five 2-criteria optimization problems results using 9 design variables.

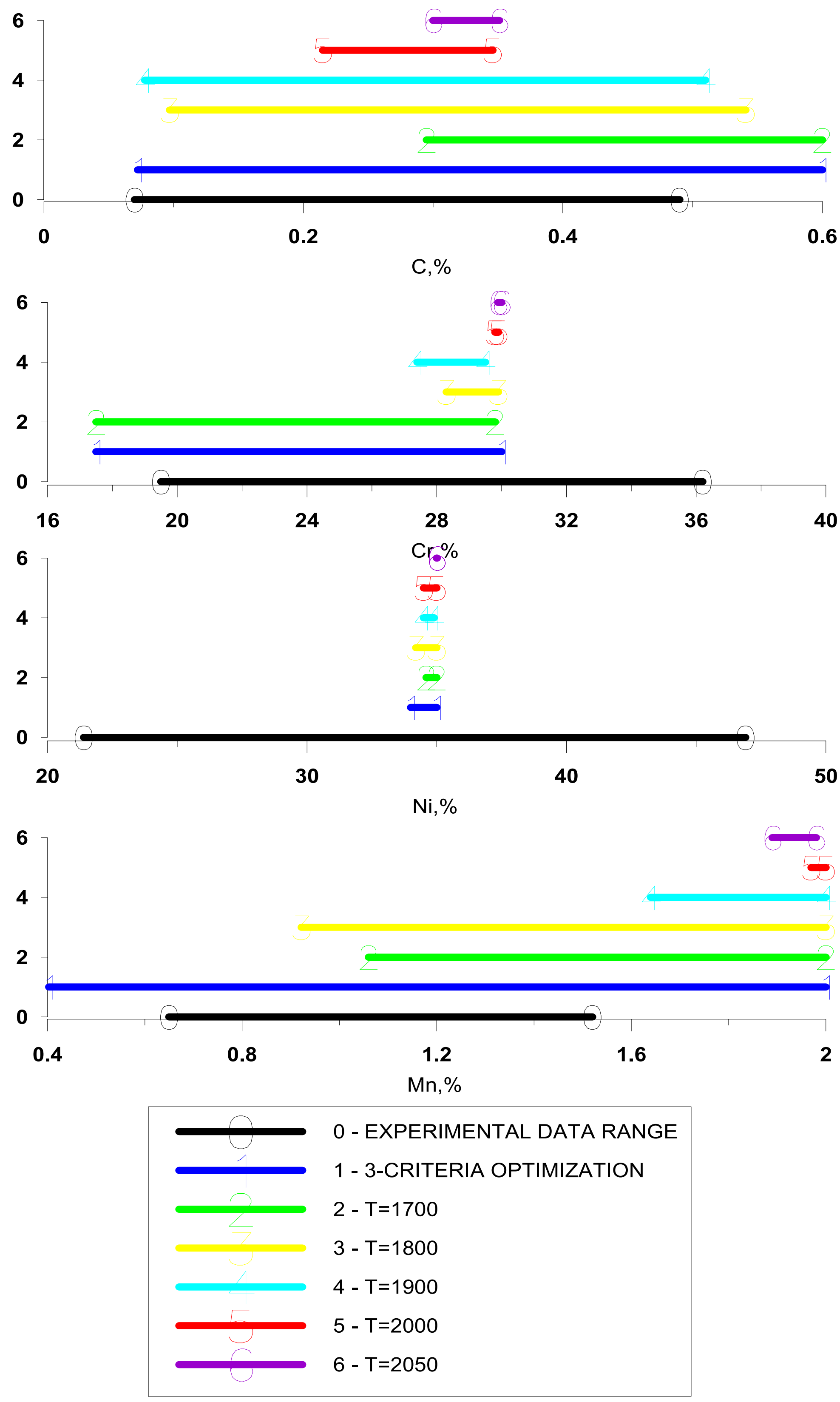


Fig. 7. Boundaries of variable parameters for sets of Pareto optimal solutions with 9 design variables.

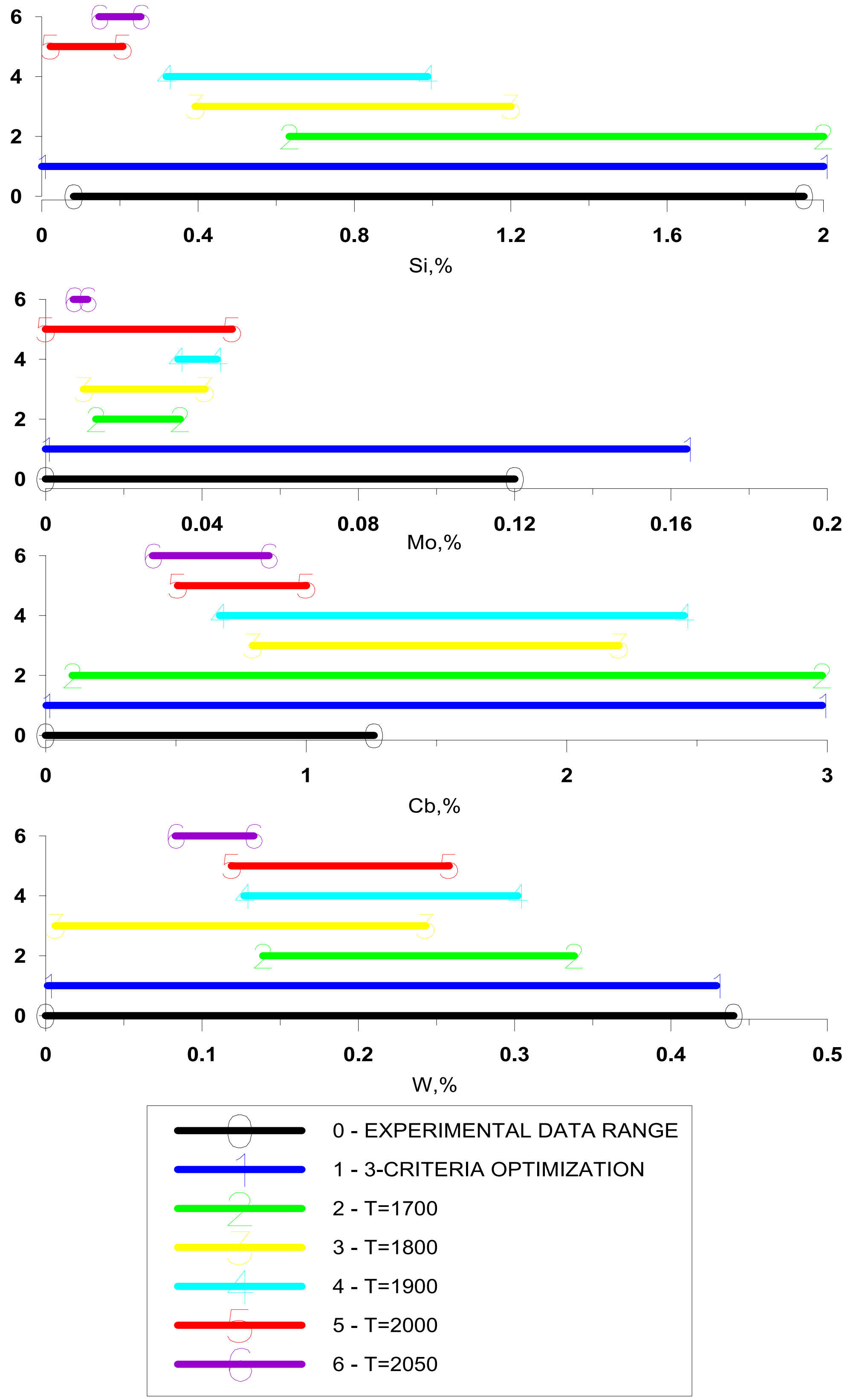


Fig. 8. Boundaries of variable parameters for sets of Pareto optimal solutions with 9 design variables.

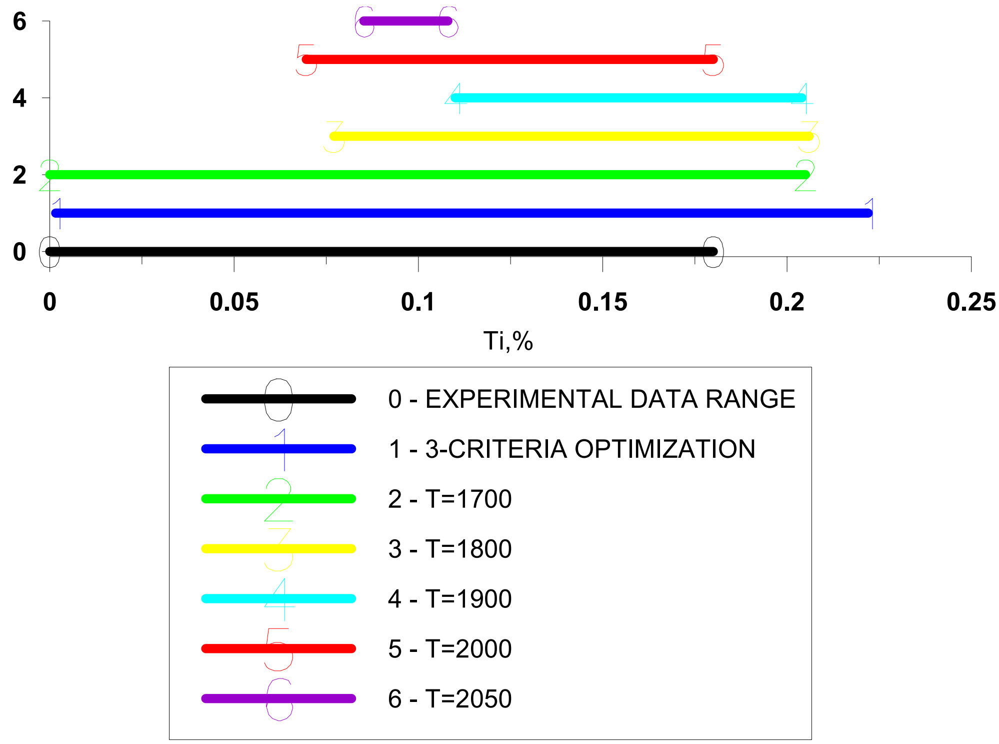


Fig. 9. Boundaries of variable parameters for sets of Pareto optimal solutions with 9 design variables.

OPTIMIZATION RESULTS FOR THE CASES WITH 8 DESIGN VARIABLES

We then repeated this optimization run (three objectives) in which we used only 9 chemical elements as independent variables:

C, Cr, Ni, Mn, Si, Mo, Cb, W

Thus, *Titanium* was deleted from the previous case with 9 variables.
We have followed the same steps during the optimization as when solving the problem with 17 variables. But, in this case there are differences:

1) The variables' ranges were changed.
In these tables you can see the previous ranges and the current ranges.

Table 1. Ranges of variation of independent variables (problem with 17 variables)

	C	**S**	**P**	**Cr**	**Ni**	**Mn**	**Si**	**Cu**	**Mo**
min	0.063	0.001	0.009	17.500	19.300	0.585	0.074	0.016	0.000
max	0.539	0.014	0.031	39.800	51.600	1.670	2.150	0.165	0.132

	Pb	**Co**	**Cb**	**W**	**Sn**	**Al**	**Zn**	**Ti**
min	0.001	0.000	0.000	0.000	0.000	0.001	0.001	0.000
max	0.006	0.319	1.390	0.484	0.007	0.075	0.015	0.198

Table 2. Ranges of variation of independent variables (problem with 8 vars.)

	C	**Cr**	**Ni**	**Mn**	**Si**	**Mo**	**Cb**	**W**
min	0.00	17.50	25.00	0.00	0.00	0.00	0.00	0.00
max	0.60	30.00	35.00	2.00	2.00	2.00	3.00	2.00

2) The accuracy of the response surfaces decreases.
The main reason of accuracy deterioration is that while decreasing the number of variables for the same experimental data set, we added the additional noise.

3-criteria optimization.

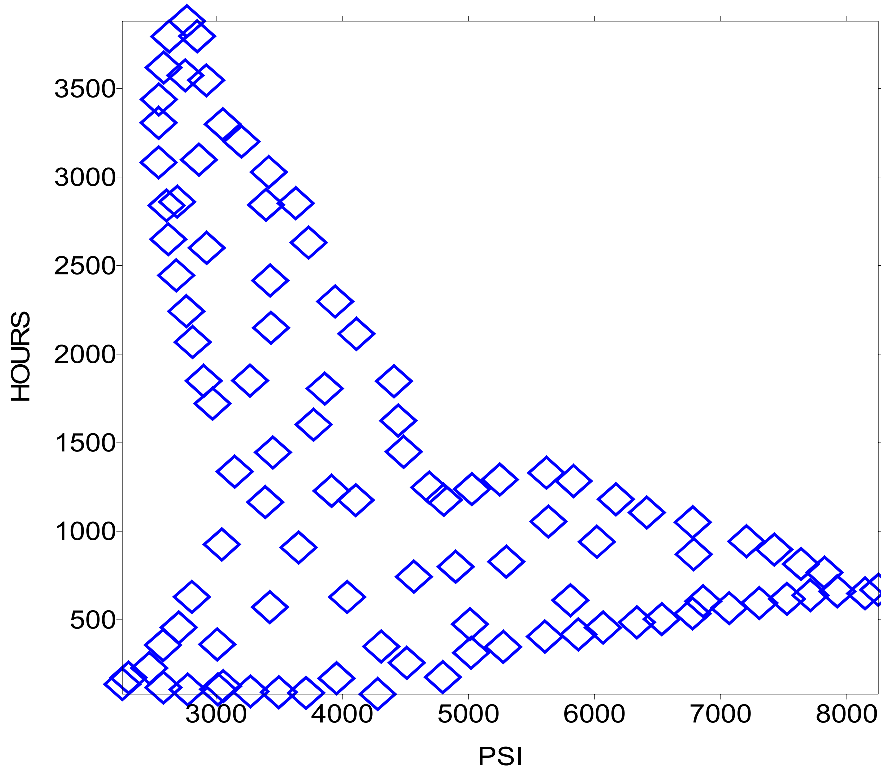
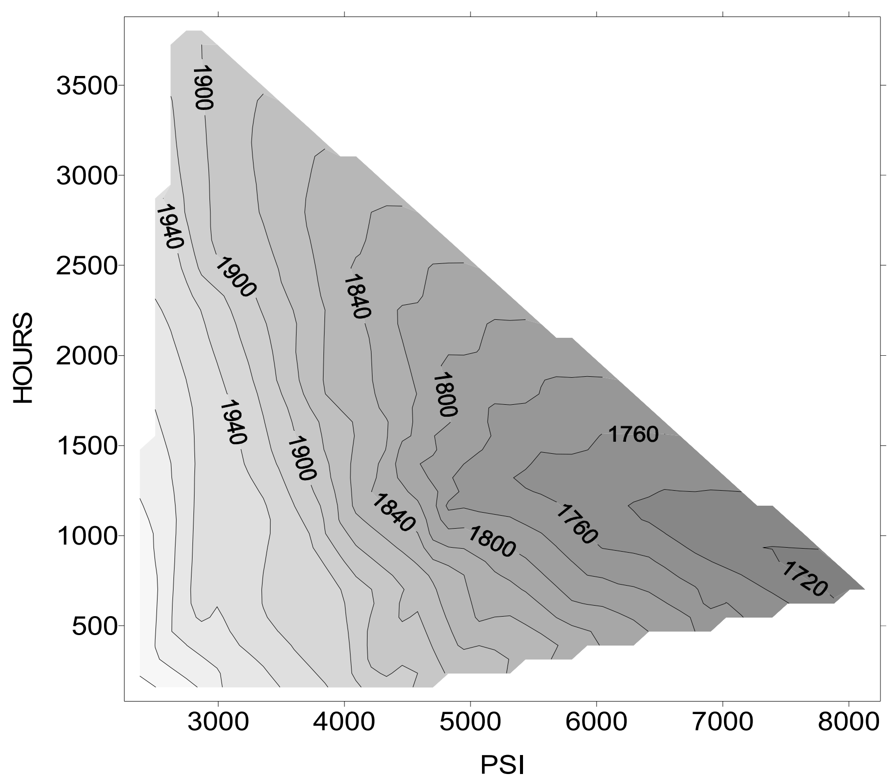


Fig. 1. Distribution of points in the objectives space using 8 design variables (chemical species).



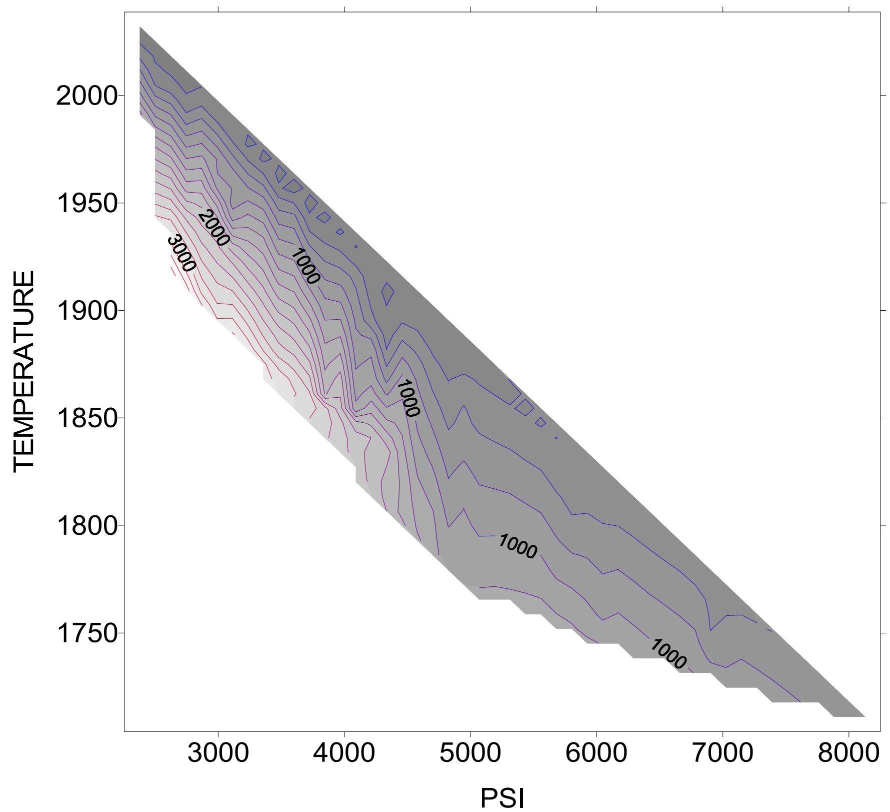
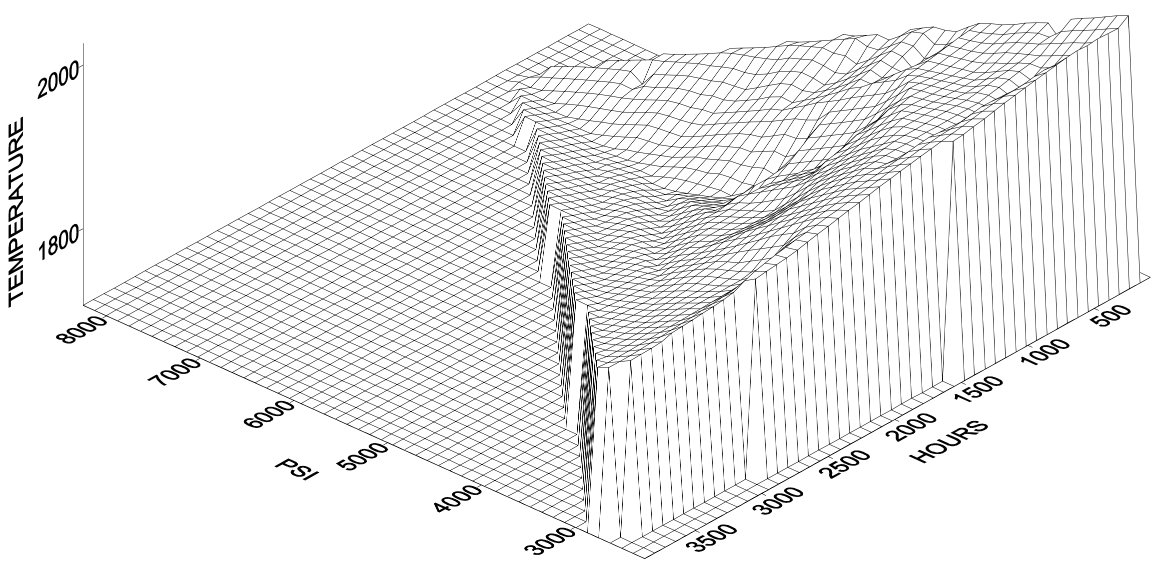


Fig. 2. Interdependence of optimization objectives for Pareto set using 8 design variables (chemical species).



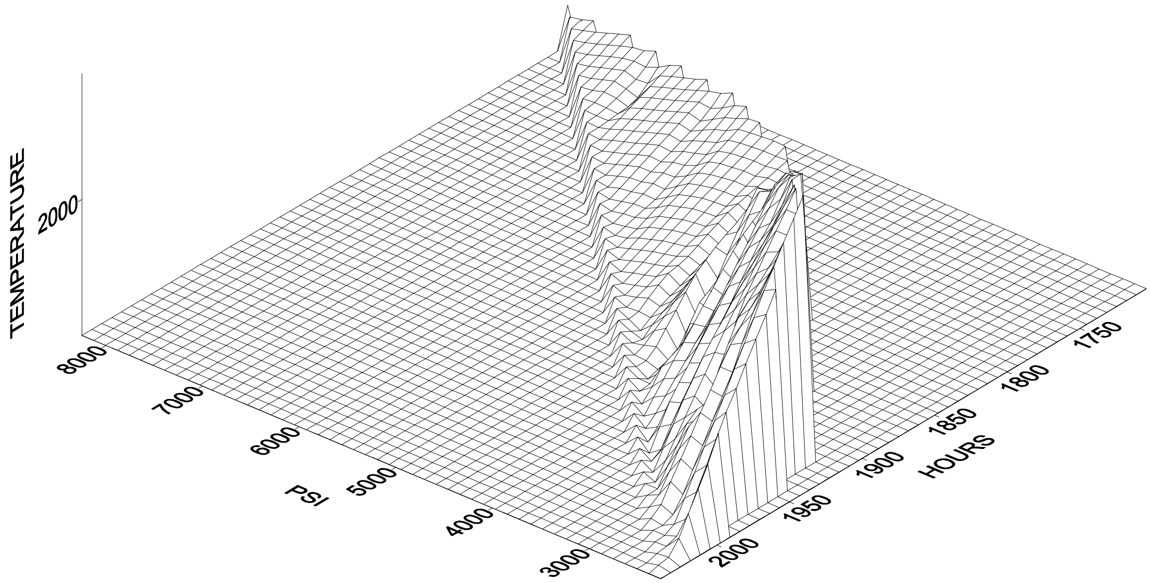


Fig. 3. Three-dimensional views of Pareto surfaces using 8 design variables (chemical species).

2-objectives optimization (tasks N2,…,N5) using 8 design variables (chemical species)

Analysis of the 3-criteria optimization results shows that there are no solutions with temperature less or equal 1600F. Because of this, we changed the value of constraint for the task N2. Constraint $T \geq 1600$ was replaced with $T \geq 1700$. Moreover, the constraint with $T \geq 2050$ has no feasible solutions in these test cases.

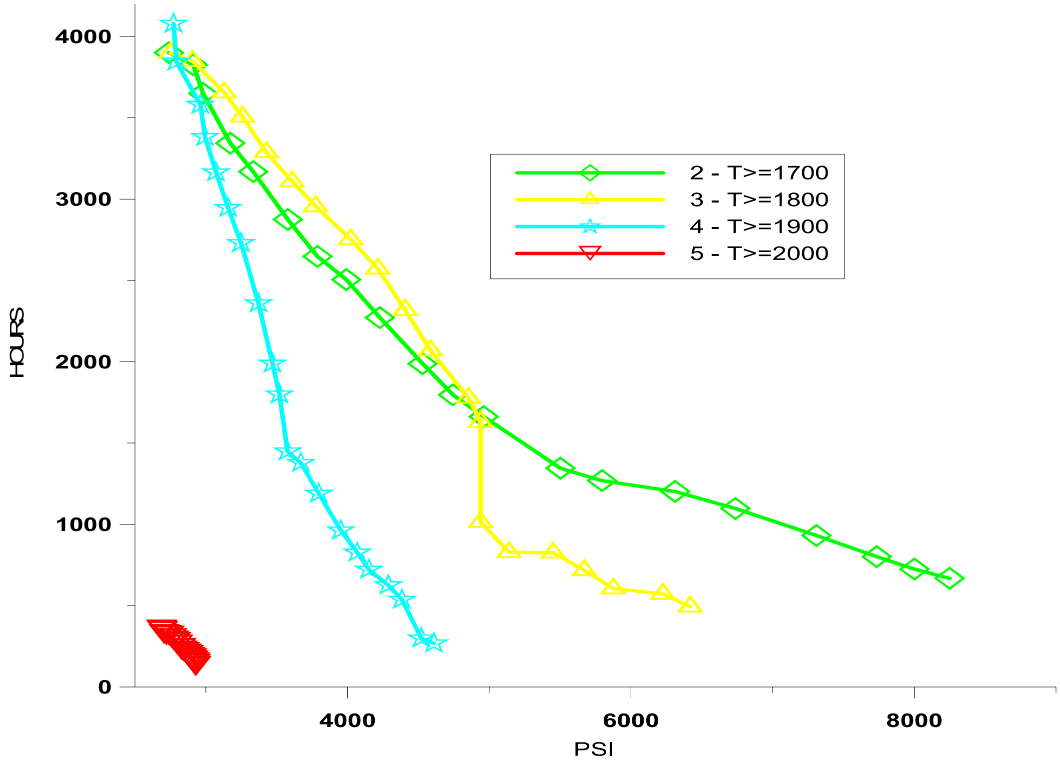


Fig.4. Pareto-optimal sets using 8 design variables (chemical species).

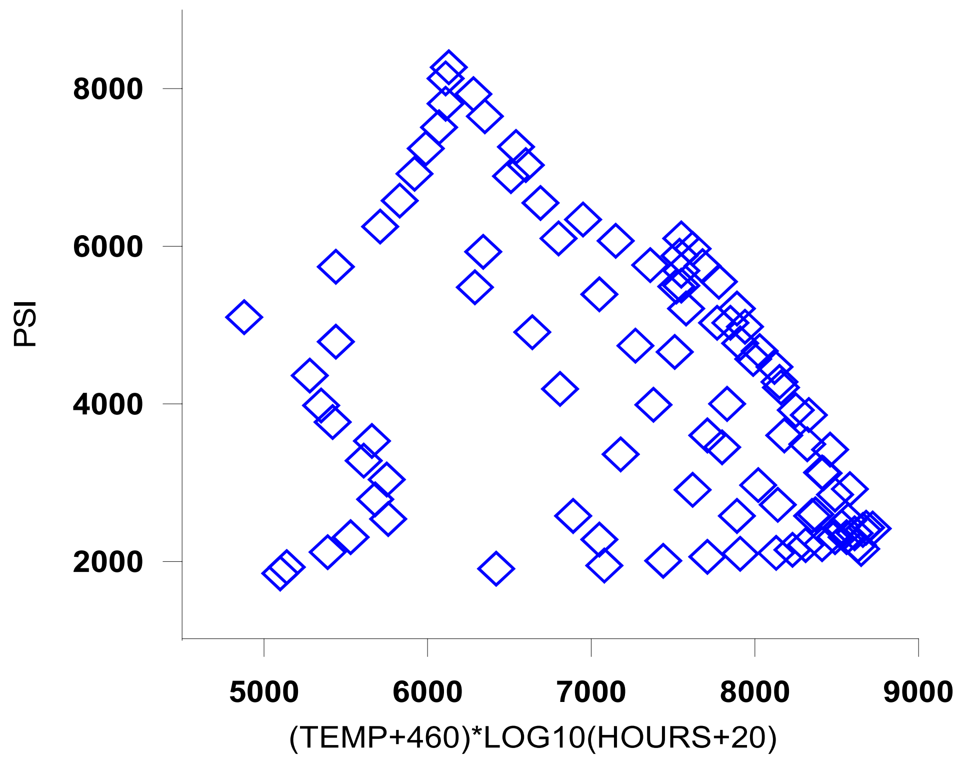


Fig. 5. Larsen-Mueller diagrams for 3-criteria optimization problems results using 8 design variables (chemical species).

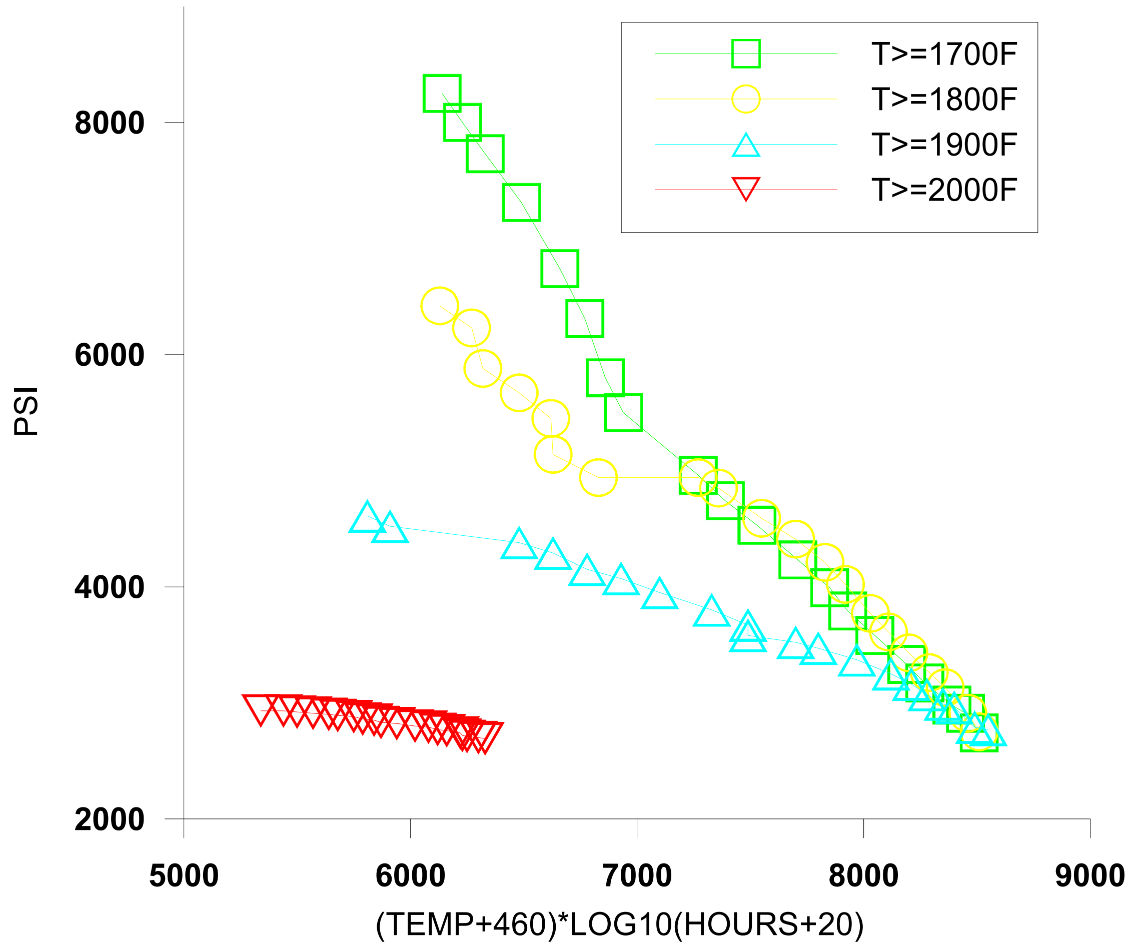


Fig. 6. Larsen-Mueller diagrams for 2-criteria optimization problems results using 8 design variables (chemical species).

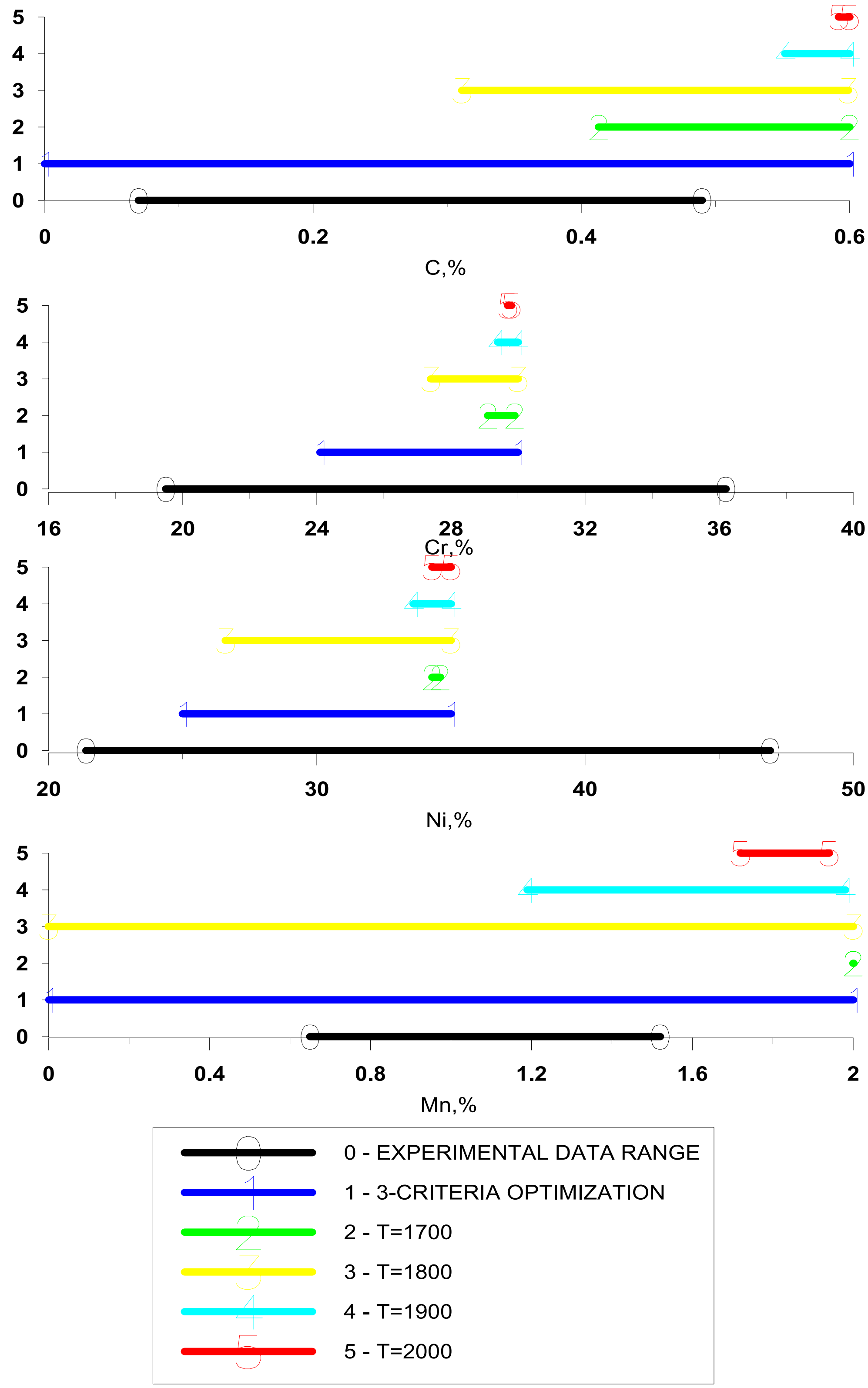


Fig. 7. Input data set and optimized ranges of chemical species using 8 design variables (chemical species).

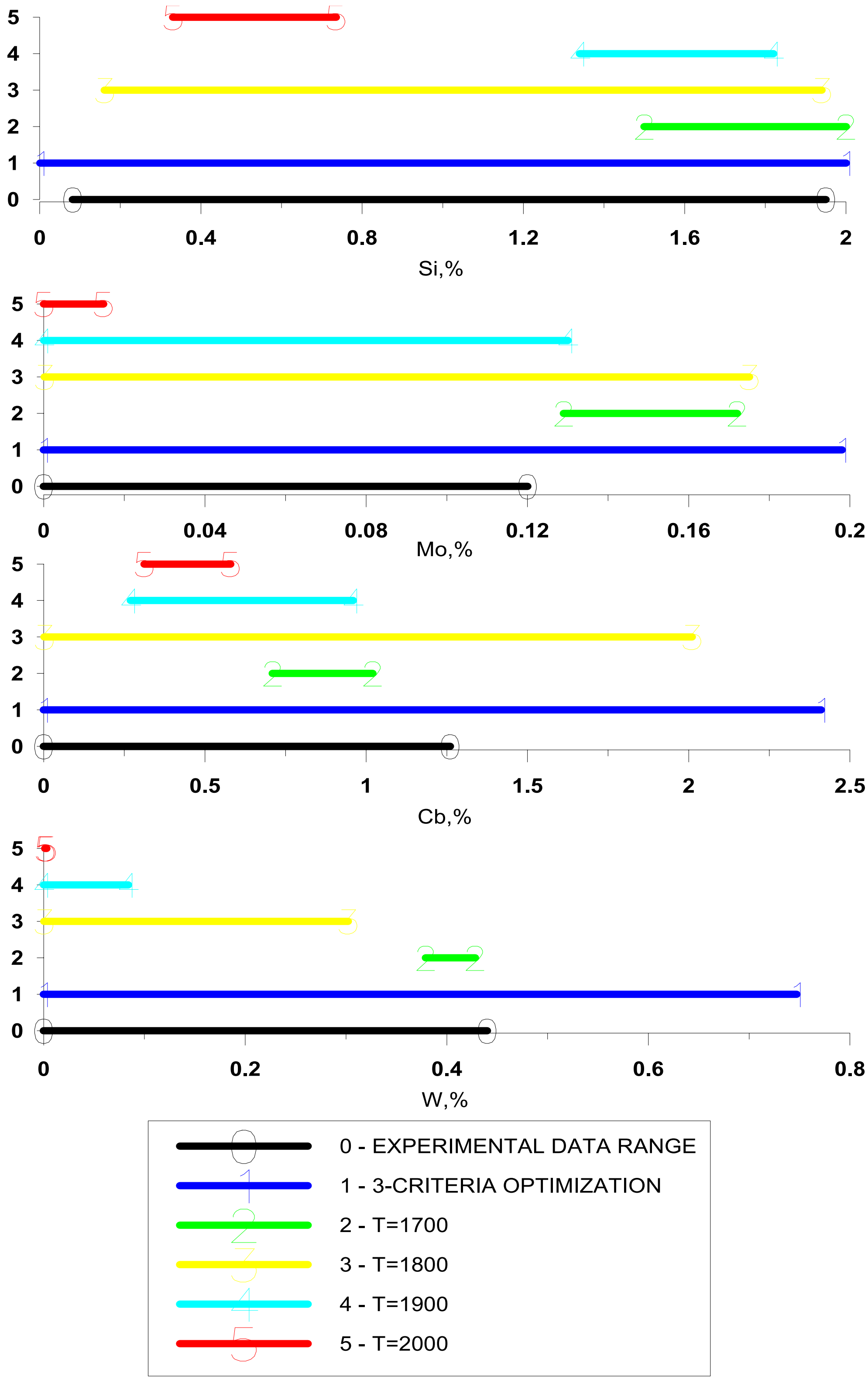


Fig. 8. Input data set and optimized ranges of chemical species using 8 design variables (chemical species).